Urochloralic acid

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 3.10 days

Global applicability domain: Outside

Local applicability domain index: 2.59e-01

Confidence level: 9.14e-01

Nearest Neighbors from the Training Set

Image not found
1-Methyl-2-propylbenzene
Measured: 12.5
Predicted: 3.17

Image not found
3-Ethyltoluene
Measured: 12.5
Predicted: 3.26

Image not found
5-Methylindan
Measured: 4.93
Predicted: 2.25

Image not found
1,3-Dimethyl-4-ethylbenzene
Measured: 24.3
Predicted: 3.89

Image not found
Propylbenzene
Measured: 24.3
Predicted: 4.02